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Interpolation of probability densities in ENDF and ENDL

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1 Summary

Suppose that we are given two probability densities $p_0(E')$ and $p_1(E')$ for the energy E' of an outgoing particle, $p_0(E')$ corresponding to energy E_0 of the incident particle and $p_1(E')$ corresponding to incident energy E_1 . If $E_0 < E_1$, our problem is how to define $p_\alpha(E')$ for intermediate incident energies

$$E_\alpha = (1 - \alpha)E_0 + \alpha E_1 \quad (1)$$

with $0 < \alpha < 1$. In this note I consider three ways to do it. I begin with unit-base interpolation, which is standard in ENDL and is sometimes used in ENDF. I then describe the equiprobable bins used by some Monte Carlo codes. I close with a discussion of interpolation by corresponding-points, which is commonly used in ENDF.

2 Why this interpolation is an issue

What we have to be careful of is to ensure that our interpolation method preserves the normalization

$$\int p(E, E') dE' = 1 \quad (2)$$

for all incident energies $E_0 < E < E_1$.

To see why the normalization (2) might be a problem consider the following “reasonable” example. Suppose that the energy densities are flat for two incident energies $E_0 < E_1$,

$$p_0(E') = 1, \quad 0 \leq E' \leq 1$$

and

$$p_1(E') = 1/2, \quad 0 \leq E' \leq 2.$$

See Fig. 1.

We don’t want to take a simple average of these densities. At incident energy

$$E_{1/10} = \frac{1}{10}(9E_0 + E_1),$$

for example, because this would give the density shown in Fig. 2. The trouble is that for incident energy close to E_0 we immediately get a positive probability density on the whole interval $1 < E' < 2$.

Another bad idea is to mindlessly interpolate both the probability densities and the lengths of the E' intervals. For the example shown in Fig. 1 this would give

$$p_{1/2}(E') = 3/4, \quad 0 \leq E' \leq 3/2.$$

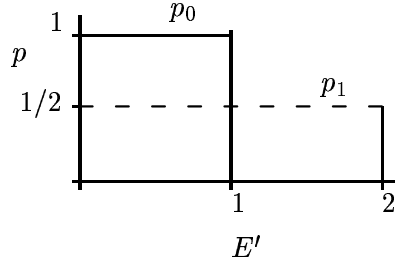


Fig. 1. Distributions for E_0 and E_1 .

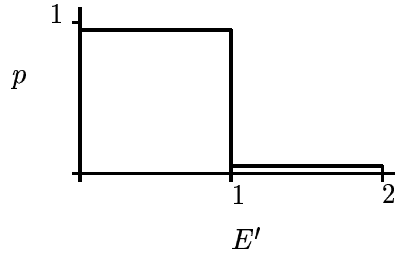


Fig. 2. Straight interpolation.

at

$$E_{1/2} = \frac{1}{2}(E_0 + E_1),$$

This density has the wrong normalization

$$\int p_{1/2}(E') dE' = 9/8.$$

In this note I illustrate three better interpolation methods using as an example the probability densities shown in Fig. 3,

$$p_0(E') = \begin{cases} 4E', & \text{for } 0 \leq E' < 1/2, \\ 4(1 - E'), & \text{for } 1/2 < E' \leq 1 \end{cases} \quad (3)$$

and

$$p_1(E') = \begin{cases} E'/2, & \text{for } 0 \leq E' < 1, \\ \frac{2}{3} - \frac{E'}{6}, & \text{for } 1 < E' \leq 4. \end{cases} \quad (4)$$

The motivation for this example, besides being simple, is that the higher-energy incident particle gives a higher-energy peak in the probability density for the energy of the outgoing particle, and it also gives a longer tail.

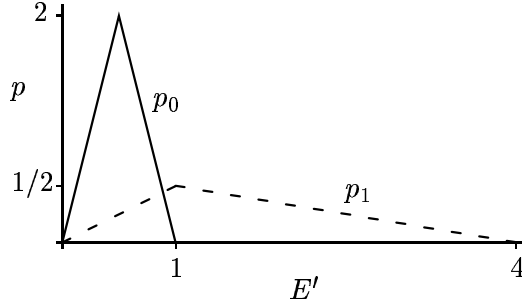


Fig. 3. Example distributions

3 Unit-base interpolation

Unit-base interpolation is defined in the Omega manual [1] on pages VI-19 to VI-22. The idea behind unit-base interpolation is that the total probability remains 1 if the interpolation is done on a fixed interval $0 \leq \eta \leq 1$. Therefore, if we have a probability density $p(E')$ defined on an energy interval $E'_{\min} \leq E' \leq E'_{\max}$, we make the change of variable

$$E' = E'_{\min} + (E'_{\max} - E'_{\min})\eta \quad (5)$$

with $0 \leq \eta \leq 1$, and we work with the scaled density

$$\Pi(\eta) = (E'_{\max} - E'_{\min})p(E'_{\min} + (E'_{\max} - E'_{\min})\eta). \quad (6)$$

This mapping maintains the normalization

$$\int_0^1 \Pi(\eta) d\eta = \int_{E'_{\min}}^{E'_{\max}} p(E') dE' = 1.$$

I now show that the unit-base mapping (6) gets the normalization right under interpolation. Suppose that we have two probability densities $\Pi_0(\eta)$ and $\Pi_1(\eta)$ both on the interval $0 \leq \eta \leq 1$ and both normalized

$$\int_0^1 \Pi_j(\eta) d\eta = 1, \quad j = 0, 1.$$

For $0 < \alpha < 1$ we define the interpolated unit-base probability as

$$\Pi_\alpha(\eta) = (1 - \alpha)\Pi_0(\eta) + \alpha\Pi_1(\eta). \quad (7)$$

It is clear that

$$\int_0^1 \Pi_\alpha(\eta) d\eta = (1 - \alpha) + \alpha = 1.$$

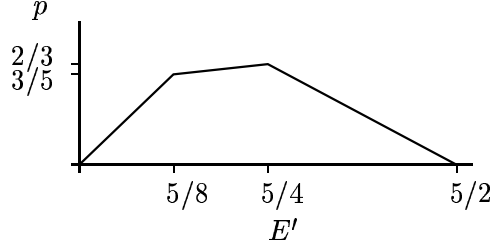


fig. 4. Interpolated by unit base

So, the normalization does come out right. To get the interpolated probability density $p_\alpha(E')$ it remains only to interpolate the energy intervals (E'_{\min}, E'_{\max}) and to invert the mapping (6). For the densities p_0 and p_1 of (3-4) shown in Fig. 3 the unit-base interpolation at $\alpha = 1/2$ is given in Fig. 4.

In order to understand why the graph in Fig. 4 looks as it does, it is useful to investigate unit-base interpolation in the original (E, E') energy space. It is clear that the length of the E' energy interval

$$L = E'_{\max} - E'_{\min}$$

plays a determining role in the mapping (6). Let L_0 denote the length of the E' energy interval for the probability density p_0 and L_1 the length of the E' energy interval for p_1 . At the intermediate incident energy E_α (1) the length is

$$L_\alpha = (1 - \alpha)L_0 + \alpha L_1.$$

With this notation the unit-base interpolation (7) takes the form

$$L_\alpha p_\alpha(E'_\alpha) = (1 - \alpha)L_0 p_0(E'_0) + \alpha L_1 p_1(E'_1). \quad (8)$$

The energies E'_α for $0 \leq \alpha \leq 1$ used in (8) are those obtained from (5) for fixed η ,

$$E'_\alpha = E'_{\min, \alpha} + L_\alpha \eta.$$

For the densities p_0 and p_1 of (3-4) this interpolation is to be done along the diagonal lines in Fig. 5. In this figure the top of the trapezoid T_1 is generated by the discontinuity in the derivative of p_1 at $E' = 1$, and the top of trapezoid T_2 is generated by the discontinuity in the derivative of p_0 at $E' = 1/2$. For $p_{1/2}$ shown in Fig. 4 the region $0 < E' < 5/8$ lies in trapezoid T_1 , the region $5/8 < E' < 5/4$ lies in trapezoid T_2 , and the region $5/4 < E' < 5/2$ lies in trapezoid T_3 . It is also significant that for each of the trapezoids T_1 , T_2 , and T_3 the ratios of the lengths of the two vertical sides is the same, namely L_1/L_0 .

4 Equiprobable bins

For a probability density $p(E')$ on an energy range $E_{\min} \leq E' \leq E_{\max}$ suppose that we want N equiprobable bins, with N a positive integer. These bins are the intervals

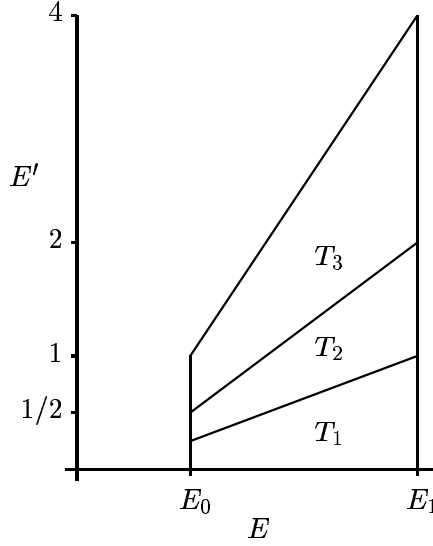


Fig. 5. Unit-base interpolation in energy space

delimited by the numbers ϵ_j such that

$$\int_{E_{\min}}^{\epsilon_j} p(E') dE' = \frac{j}{N} \quad (9)$$

for $j = 0, 1, \dots, N$. It is clear that $\epsilon_0 = E'_{\min}$, and it follows from the normalization that $\epsilon_N = E'_{\max}$.

Warning. The condition on the probability density is only that $p(E') \geq 0$ on the energy range $E_{\min} \leq E' \leq E_{\max}$. If it should happen that $p(E') = 0$ on a subinterval, then the values ϵ_j defined by (9) may not be uniquely determined. This could occur, for example, if $p(E')$ is the probability density of a set of discrete gamma lines. It is not a good idea to use interpolation by equiprobable bins in such situations.

For interpolation by equiprobable bins between a probability density $p_0(E')$ at incident energy E_0 and density $p_1(E')$ at incident energy E_1 we use (9) to calculate the bin edges $\epsilon_j(0)$ for p_0 and $\epsilon_j(1)$ for p_1 . For an intermediate incident energy

$$E_\alpha = (1 - \alpha)E_0 + \alpha E_1$$

with $0 < \alpha < 1$ we use interpolated bin edges

$$\epsilon_j(\alpha) = (1 - \alpha)\epsilon_j(0) + \alpha\epsilon_j(1).$$

On the interval $\epsilon_{j-1}(\alpha) < E' < \epsilon_j(\alpha)$ we define the probability density $p_\alpha(E')$ to be

$$p_\alpha(E') = \frac{1}{N(\epsilon_j(\alpha) - \epsilon_{j-1}(\alpha))}.$$

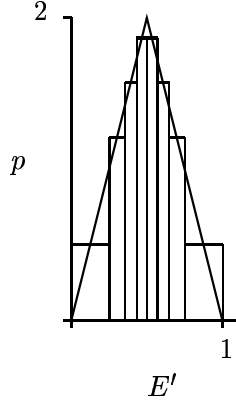


Fig. 6. Equiprobable bins for p_0

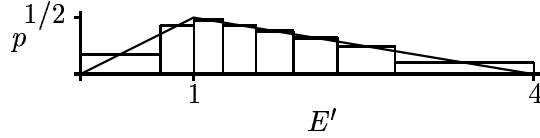


Fig. 7. Equiprobable bins for p_1

This value is chosen to make

$$\int_{\epsilon_{j-1}(\alpha)}^{\epsilon_j(\alpha)} p_\alpha(E') dE' = \frac{1}{N}.$$

With $N = 8$ the equiprobable bins for the probability density $p_0(E')$ of (3) are shown in Fig. 6, and the equiprobable bins for the density $p_1(E')$ of (4) are shown in Fig. 7. The interpolated equiprobable bins for $p_{1/2}(E')$ are shown in Fig. 8.

The (E, E') energy space version of this interpolation is illustrated in Fig. 9. In fact, we are doing unit-base interpolation within each trapezoid in this figure, but now L_0 and L_1 in equation (8) refer to the lengths of the vertical edges of the trapezoids. Hence, the ratio L_1/L_0 differs from one trapezoid to another.

It is interesting to investigate the continuum limit of equiprobable bin interpolation as $N \rightarrow \infty$. For interpolation of the densities $p_0(E')$ of (3) and $p_1(E')$ of (4) this limit is shown as the continuous curve in Fig. 8. In this discussion we need to be careful of the mathematical terminology. Up to this point we have worked only with *probability densities* $p(E')$, namely, nonnegative functions such that

$$\int_{E'_{\min}}^{E'_{\max}} p(E') dE' = 1.$$

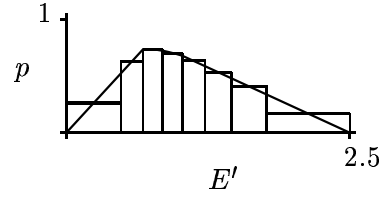


Fig. 8. Equiprobable bins for $p_{1/2}$

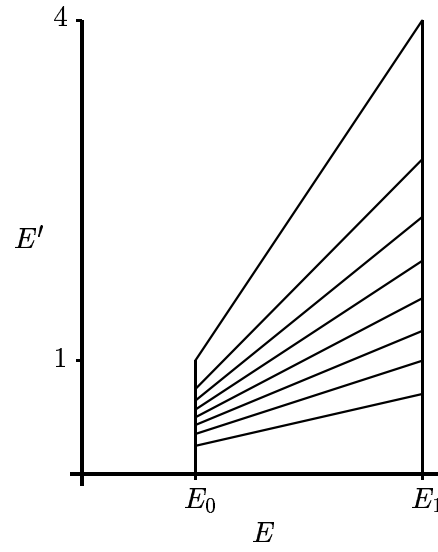


Fig. 9. The view in energy space

The analysis of equiprobable bin interpolation is based on the corresponding *distribution function* $F(E')$ defined by the integral

$$F(E') = \int_{E'_{\min}}^{E'} p(E'') dE''.$$

In fact, it follows from (9) that the equiprobable bin edges ϵ_j for $j = 0, 1, \dots, N$ are obtained from the inverse to the distribution function,

$$\epsilon_j = F^{-1} \left(\frac{j}{N} \right).$$

In view of the warning given above, I assume in this discussion that $F(E')$ is strictly increasing

$$F(E'_2) > F(E'_1) \quad \text{whenever } E'_{\min} \leq E'_1 < E'_2 \leq E'_{\max}. \quad (10)$$

This condition implies that $F^{-1}(y)$ is uniquely defined for $0 \leq y \leq 1$.

With this background, we see that the continuum version of interpolation by equiprobable bins proceeds by the following steps.

1. Given probability densities $p_0(E')$ for incident energy E_0 and $p_1(E')$ for incident energy E_1 , form the corresponding distribution functions $F_0(E')$ and $F_1(E')$.
2. Solve the equations $y = F_0(E')$ and $y = F_1(E')$ to determine the inverse distribution functions $E' = F_0^{-1}(y)$ and $E' = F_1^{-1}(y)$ on $0 \leq y \leq 1$.
3. For $0 < \alpha < 1$ the interpolated inverse distribution function $F_\alpha^{-1}(y)$ is defined as

$$F_\alpha^{-1}(y) = (1 - \alpha)F_0^{-1}(y) + \alpha F_1^{-1}(y).$$

4. Get the interpolated distribution function $y = F_\alpha(E')$ by solving the equation $E' = F_\alpha^{-1}(y)$.
5. Differentiate to obtain the interpolated probability density

$$p_\alpha(E') = \frac{d}{dE'} F_\alpha(E').$$

Interpolation by equiprobable bins is simply a finite-difference approximation to this algorithm.

Let's illustrate these ideas by applying them to the densities p_0 and p_1 of (3-4). The distribution function $F_0(E')$ for $p_0(E')$ is obtained by integrating (3),

$$F_0(E') = \begin{cases} 2E'^2 & \text{for } 0 \leq E' \leq 1/2, \\ -1 + 4E' - 2E'^2 & \text{for } 1/2 \leq E' \leq 1. \end{cases}$$

Note that in the equation $y = F_0(E')$ the interval $0 \leq E' \leq 1/2$ corresponds to $0 \leq y \leq 1/2$ and $1/2 \leq E' \leq 1$ corresponds to $1/2 \leq y \leq 1$. In inverting $y = F_0(E')$ we take the physically relevant square roots,

$$E' = F_0^{-1}(y) = \begin{cases} \sqrt{\frac{y}{2}} & \text{for } 0 \leq y \leq 1/2, \\ 1 - \sqrt{\frac{1-y}{2}} & \text{for } 1/2 \leq y \leq 1. \end{cases} \quad (11)$$

If we apply the same operations to the probability density $p_1(E')$ given by (4), we get the distribution function

$$F_1(E') = \begin{cases} \frac{E'^2}{4} & \text{for } 0 \leq E' \leq 1, \\ -\frac{1}{3} + \frac{2E'}{3} - \frac{E'^2}{12} & \text{for } 1 \leq E' \leq 4. \end{cases}$$

For $y = F_1(E')$ the interval $0 \leq E' \leq 1$ corresponds to $0 \leq y \leq 1/4$ and the interval $1 \leq E' \leq 4$ corresponds to $1/4 \leq y \leq 1$. The inverse distribution function is given by

$$E' = F_1^{-1}(y) = \begin{cases} \sqrt{2y} & \text{for } 0 \leq y \leq 1/4, \\ 4 - \sqrt{3(1-y)} & \text{for } 1/4 \leq y \leq 1. \end{cases} \quad (12)$$

Let us interpolate half way between these inverse distribution functions,

$$F_{1/2}^{-1}(y) = \frac{1}{2}(F_0^{-1}(y) + F_1^{-1}(y)). \quad (13)$$

It is clear from (11-12) that this function is defined on the interval $0 \leq y \leq 1$ and that it is given by 3 different formulas, depending on whether $0 \leq y \leq 1/4$ or $1/4 \leq y \leq 1/2$ or $1/2 \leq y \leq 1$. Let us examine these regions one at a time.

On the interval $0 \leq y \leq 1/4$ equation (13) takes the form

$$E' = \left(1 + \frac{\sqrt{2}}{4}\right) \sqrt{y}. \quad (14)$$

The range of E' values is from

$$E' = 0 \quad \text{for} \quad y = 0$$

to

$$E' = \frac{4 + \sqrt{2}}{8} \quad \text{for} \quad y = \frac{1}{4}.$$

Upon solving (14) for y , we get the distribution function

$$F_{1/2}(E') = \left(\frac{4}{4 + \sqrt{2}}\right)^2 E'^2 \quad \text{for} \quad 0 \leq E' \leq \frac{4 + \sqrt{2}}{8}.$$

The probability density is the derivative

$$p_{1/2}(E') = \left(\frac{4}{4 + \sqrt{2}} \right)^2 2E' \quad \text{for } 0 \leq E' \leq \frac{4 + \sqrt{2}}{8}.$$

The algebra is more complicated for $1/4 \leq y \leq 1/2$ because from (13) we obtain the equation

$$F_{1/2}^{-1}(y) = \frac{1}{2} \sqrt{\frac{y}{2}} + 2 - \sqrt{3(1-y)}.$$

In particular, $y = 1/2$ corresponds to

$$E' = F_{1/2}^{-1}(1/2) = \frac{9}{4} - \frac{\sqrt{3}}{2}.$$

It is possible to solve $E' = F_{1/2}^{-1}(y)$ for $y = F_{1/2}(E')$, but I choose not to do it.

For $1/2 \leq y \leq 1$ we find from (13) that

$$E' = F_{1/2}^{-1}(y) = \frac{5}{2} - \left(\frac{\sqrt{2}}{4} + \sqrt{3} \right) \sqrt{1-y}.$$

With the notation

$$\beta = \frac{\sqrt{2}}{4} + \sqrt{3},$$

we can easily solve this equation for y to get

$$y = F_{1/2}(E') = \frac{1}{\beta^2} \left(\frac{5}{2} - E' \right)^2$$

for

$$\frac{9}{4} - \frac{\sqrt{3}}{2} \leq E' \leq \frac{5}{2}.$$

The derivative of $F_{1/2}(E')$ is the probability density

$$p_{1/2}(E') = \frac{2}{\beta^2} \left(\frac{5}{2} - E' \right).$$

5 Interpolation by corresponding points

The ENDF documentation on interpolation by corresponding points [2] page 34 is not entirely clear, so I give here my interpretation.

In the method of corresponding points the probability densities $p(E, E')$ are piecewise linear in the energy E' of the outgoing particle, and the same number N of data points (E', p) are to be given for each incident energy E . Interpolation by corresponding points is by unit-base interpolation (8) between adjacent points in the table. But the lengths L_0 and L_1 used in the interpolation are local.

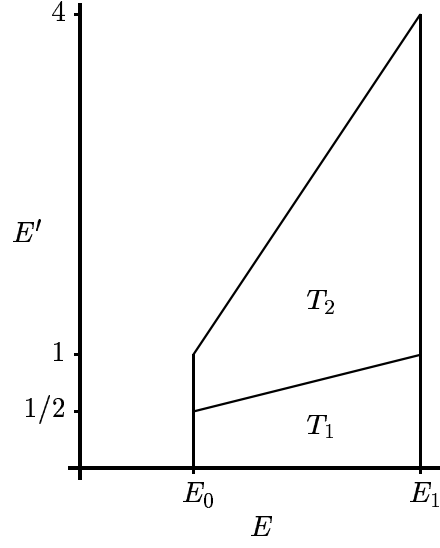


Fig. 10. Corresponding points for our example

	$E = E_0$		$E = E_1$	
n	E'	p	E'	p
1	0	0	0	0
2	1/2	2	1	1/2
3	1	0	4	0

Table 1. Corresponding points

I illustrate the process with a simple example with $N = 3$ based on the probability densities (3-4) shown in Fig. 3. The corresponding data points are the vertices of the triangles in Fig. 3, and they are given in Table 1.

These corresponding points determine trapezoids T_1 and T_2 in energy space, as displayed in Fig. 10. Let's see what the corresponding points interpolation gives along the bottom of the trapezoid T_2 at the incident energy

$$E_{1/2} = \frac{1}{2}(E_0 + E_1).$$

The lengths of the vertical sides of T_2 are

$$L_0 = \frac{1}{2} \quad \text{and} \quad L_1 = 3,$$

and the average length is

$$L_{1/2} = \frac{7}{4}.$$

Unit-base interpolation (8) in T_2 therefore takes the form

$$\frac{7}{4}p_{1/2}(3/4) = \frac{1}{2} \left(\frac{1}{2}^2 + 3\frac{1}{2} \right).$$

Consequently, we find that

$$p_{1/2}(3/4) = \frac{5}{7}$$

as viewed from T_2 .

The value of $p_{1/2}(3/4)$ as viewed from T_1 is different because for T_1 the ratio of the lengths of the vertical sides

$$\frac{L_1}{L_0} = 2$$

is different from the corresponding ratio for T_2

$$\frac{L_1}{L_0} = 6.$$

This explains the jump discontinuity shown in Fig. 11. The full set of interpolated values is given in Table 2.

Another problem with interpolation by corresponding points is that the lengths of the data columns may not be the same. For example, it is not at all clear how to pair up the data points in Table 3. Table 3 was obtained by inserting an extra point into the last 2 columns of Table 1.

My interpretation of interpolation by corresponding points is to extend the short list by repeating the last pair, as in Table 4.

This extension is shown in energy space in Fig. 12. One peculiarity of extending the corresponding points by a triangle, as I have done with T_3 is that from the T_3 side of the line from A to B the probability density $p_\alpha(E')$ is the constant value that it takes at B .

The lack of a formal extension rule for different numbers of corresponding points is significant, because every ENDF/B-VII and JEFF evaluation which calls for interpolation by corresponding points happens to have different numbers of points.

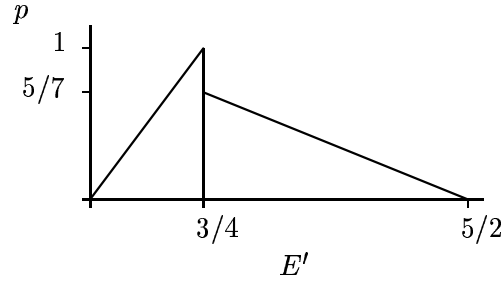


Fig. 11. Interpolation by corresponding points

	$E = E_0$		$E = E_{1/2}$		$E = E_1$	
n	E'	p	E'	p	E'	p
1	0	0	0	0	0	0
2	1/2	2	3/4	1	1	1/2
2	1/2	2	3/4	5/7	1	1/2
3	1	0	5/2	0	4	0

Table 2. Interpolation by corresponding points

	$E = E_0$		$E = E_1$	
n	E'	p	E'	p
1	0	0	0	0
2	1/2	2	1	1/2
3	1	0	3	1/6
4			4	0

Table 3. Unmatched points

	$E = E_0$		$E = E_{1/2}$		$E = E_1$	
n	E'	p	E'	p	E'	p
1	0	0	0	0	0	0
2	1/2	2	3/4	1	1	1/2
2	1/2	2	3/4	4/5	1	1/2
3	1	0	2	2/15	3	1/6
3	1	0	2	1/6	3	1/6
4	1	0	5/2	0	4	0

Table 4. Extended table.

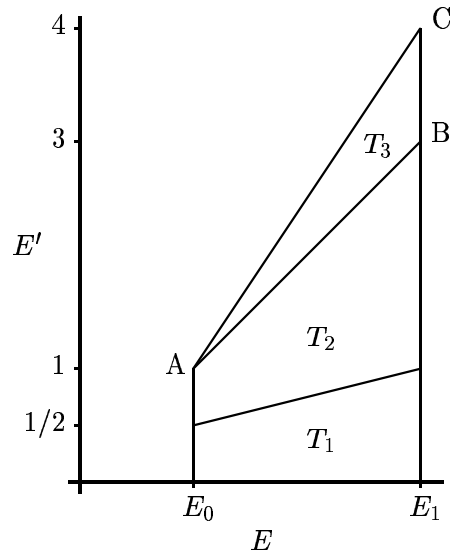


Fig. 12. A triangular extension

6 Comments

The principal disadvantage of unit-base interpolation is that its division of the domain in energy space into trapezoids with equal ratios of the vertical sides L_1/L_0 as in Fig. 5 may not be consistent with the physics of the probability densities. Interpolation by equiprobable bins makes more sense to me physically, but it also has difficulties. As seen in Fig. 8, the continuum limit gives a very reasonable interpolation, but for any finite number of bins the approximation is poor in regions of low probability density. Another drawback of equiprobable bins is that the process is undefined if $p(E') = 0$ on an interval interior to its domain of definition. This is a violation of the condition (10) which is necessary for the method to work.

The primary difficulty with the method of interpolation by corresponding points is the question of what to do when the number of points is not the same. I have made what seems to me to be a reasonable guess. Another aspect to be aware of is that the method generates discontinuities in the interpolated probability density as in Fig. 11 when the ratio L_1/L_0 changes from one energy trapezoid to the next.

References

- [1] R. J. Howerton, R. E. Dye, P. C. Giles, J. R. Kimlinger, S. T. Perkins, and E. F. Plechaty, “Omega: a Cray 1 executive code for LLNL nuclear data libraries”, Report UCRL-50400 Vol. 25, Lawrence Livermore National Laboratory, Livermore, California, 1983.
- [2] M. Herman, ed., “ENDF-102 ENDF-6 data formats and procedures for the evaluated nuclear data file ENDF-VII”, Informal report BNL-NCS-44945-01/04-Rev., National Nuclear Data Center, Brookhaven National Laboratory, Upton, New York. 2005.